

1 Particle Kalman Filtering: A Nonlinear Bayesian
2 Framework for Ensemble Kalman Filters

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Abstract

This paper investigates an approximation scheme of the optimal nonlinear Bayesian filter based on the Gaussian mixture representation of the state probability distribution function. The resulting filter is similar to the particle filter, but is different from it in that, the standard weight-type correction in the particle filter is complemented by the Kalman-type correction with the associated covariance matrices in the Gaussian mixture. We show that this filter is an algorithm in between the Kalman filter and the particle filter, and therefore is referred to as the particle Kalman filter (PKF).

In the PKF, the solution of a nonlinear filtering problem is expressed as the weighted average of an “ensemble of Kalman filters” operating in parallel. Running an ensemble of Kalman filters is, however, computationally prohibitive for realistic atmospheric and oceanic data assimilation problems. For this reason, we consider the construction of the PKF through an “ensemble” of ensemble Kalman filters (EnKFs) instead, and call the implementation the particle EnKF (PEnKF). We show that different types of the EnKFs can be considered as special cases of the PEnKF. Similar to the situation in the particle filter, we also introduce a re-sampling step to the PEnKF in order to reduce the risk of weights collapse and improve the performance of the filter. Numerical experiments with the strongly nonlinear Lorenz-96 model are presented and discussed.

1 Introduction

Estimating the state of the atmosphere and the ocean has long been one of the main goals of modern science. Data assimilation, which consists of combining data and dynamical models to determine the best possible estimate of the state of a system, is now recognized as the best approach to tackle this problem (Ghil and Malanotte-Rizzoli, 1991). The strongly nonlinear character of the atmospheric and oceanic models, combined with their important computational burden, makes data assimilation in these systems quite challenging.

Based on the Bayesian estimation theory, the optimal solution of the nonlinear data assimilation problem can be obtained from the optimal nonlinear filter (ONF) (Doucet et al., 2001). This involves the estimation of the conditional probability distribution function (*pdf*) (not necessarily Gaussian) of the system state given all available measurements up to the estimation time. Knowledge of the state *pdf* allows determining different estimates of the state, such as the minimum variance estimate or the maximum a posteriori estimate (Todling, 1999). The ONF recursively operates as a succession of a correction (or analysis) step at measurement times to correct the state (predictive) *pdf* using the Bayes' rule, and a prediction step to propagate the state (analysis) *pdf* to the time of the next available observation. Although conceptually simple, the numerical implementation of the optimal nonlinear filter can be computationally prohibitive, even for systems with few dimensions (Doucet et al., 2001). Its use with atmospheric and oceanic data assimilation problems is therefore not possible because of the huge dimension of these systems.

In recent years, two approximation schemes of the ONF have attracted the attention of researchers for their potentials to tackle nonlinear and non-Gaussian data assimilation problems. One is based on the point-mass representation (mixture of Dirac functions) of the state *pdf*, and leads to the celebrated particle filter (PF) (Doucet et al., 2001; Pham, 2001; Nakano et al., 2007; Van Leeuwen, 2003, 2009).

The other is based on the Gaussian mixture representation of the state *pdf*, and results in a filter that is in between the Kalman filter and the particle filter (Anderson and Anderson, 1999; Bengtsson et al., 2003; Chen and Liu, 2000; Hoteit et al., 2008; Luo et al., 2010; Sorenson and Alspach, 1971), as to be shown later. For this reason, we refer to this filter as the particle Kalman filter (PKF).

In terms of computational efficiency, the particle filter needs to generate large samples for a good approximation of the state *pdf*. In certain circumstances, in order to avoid weights collapse, the number of samples needs to scale exponentially with the dimension of the system in assimilation (Bengtsson et al., 2008), which may be infeasible for high-dimensional systems (Snyder et al., 2008). On the other hand, in some comparison studies (Han and Li, 2008; Nakano et al., 2007), it has been reported that the ensemble Kalman filter (EnKF) and its variants (Anderson, 2001; Bishop et al., 2001; Burgers et al., 1998; Evensen, 1994; Evensen and van Leeuwen, 1996; Houtekamer and Mitchell, 1998; Whitaker and Hamill, 2002) can achieve lower estimation errors than the particle filter given a small ensemble size. To save space, in this paper we confine ourselves to the PKF, and make performance comparison only between the PKF and the EnKF.

Using a Gaussian mixture representation of the state *pdf*, the resulting PKF consists of an ensemble of parallel nonlinear Kalman filters (Hoteit et al., 2008; Luo et al., 2010). Different variants of the Kalman filter (KF), including the extended Kalman filter (Chen and Liu, 2000; Sorenson and Alspach, 1971), the reduced-rank Kalman filter (Hoteit et al., 2008; Luo et al., 2010), the EnKF (Anderson and Anderson, 1999; Bengtsson et al., 2003), can be used to construct the PKF. The focus of this paper is to investigate the PKF that is constructed by an ensemble of parallel EnKFs. Common to all the implementations of the PKF, the mixture of normal distributions (MON) – a more general *pdf* representation than the single Gaussian *pdf* approximation in the EnKF – can be used to tackle nonlinearity and non-Gaussianity in data assimilation. On the other hand, choosing the EnKF to construct the PKF is

81 based on the consideration of computational efficiency, since the EnKF itself is a very
82 efficient algorithm for data assimilation in high dimensional systems. In this regard,
83 this work is very similar to the earlier works of Anderson and Anderson (1999) and
84 Bengtsson et al. (2003), but is different from them mainly in the following aspect.

85 In Anderson and Anderson (1999) and Bengtsson et al. (2003), the PKF was con-
86 structed without a re-sampling step. As a result, the PKF may suffer from weights
87 collapse as in the particle filter. To overcome this problem, Bengtsson et al. (2003)
88 considered a hybrid of the EnKF and the PKF, which, however, involves the computa-
89 tion of the inverses of sample covariance matrices in the “global-to-local” adjustments.
90 In doing so, it is not only computationally intensive, but also encounters singularities
91 in computing the inverses when the ensemble size is smaller than the system dimen-
92 sion, such that the sample covariances themselves are rank deficient. Therefore, it
93 is not clear how the hybrid scheme in Bengtsson et al. (2003) can be applied to the
94 scenario with the ensemble size smaller than the system dimension. For the imple-
95 mentation of the PKF scheme in this work, we introduce a re-sampling step similar
96 to those in Musso et al. (2001) and Stavropoulos and Titterton (2001) to tackle
97 weights collapse. Our experience shows that, with this re-sampling step, the PKF
98 becomes much more stable and can conduct data assimilation in the small ensemble
99 scenario, as to be demonstrated through the numerical experiments presented in this
100 work.

101 As may be of particular interest for the ensemble filtering community, we will show
102 that different EnKFs can be considered as special cases of the PEnKF following our
103 implementation. This point of view allows for a better understanding of the EnKFs’
104 behaviors and/or their differences.

105 The paper is organized as follows. The optimal nonlinear filter is first described
106 in section 2. The PKF and its ensemble implementation are discussed in section 3.
107 Results of numerical experiments with the Lorenz-96 model are presented in section
108 4. A summary of the main results and a general discussion on the potential of the

PEnKF for tackling realistic atmospheric and oceanic data assimilation problems
concludes the paper in section 5.

2 The Optimal Nonlinear Filter

Starting from a random initial condition with a known probability density function,
the optimal nonlinear filter provides the conditional density function of the system
state given all available measurements up to the estimation time. To describe the
algorithm of the optimal nonlinear filter, consider the nonlinear stochastic discrete-
time dynamical system

$$\mathbf{x}_k = \mathbf{M}_k(\mathbf{x}_{k-1}) + \boldsymbol{\eta}_k, \quad (1)$$

$$\mathbf{y}_k = \mathbf{H}_k(\mathbf{x}_k) + \boldsymbol{\epsilon}_k, \quad (2)$$

where \mathbf{x}_k is the state vector (to be estimated), of dimension n , \mathbf{y}_k is the observa-
tion vector, of dimension p , \mathbf{M}_k and \mathbf{H}_k are two continuously differentiable maps
from \mathbb{R}^n to \mathbb{R}^n and from \mathbb{R}^n to \mathbb{R}^p respectively representing the transition and the
observational operators, and $\boldsymbol{\eta}_k$ and $\boldsymbol{\epsilon}_k$ denote the dynamical and the observational
noise, respectively. We assume that $\boldsymbol{\eta}_k$ and $\boldsymbol{\epsilon}_k$ are Gaussian with zero mean and non-
singular covariance matrices \mathbf{Q}_k and \mathbf{R}_k , respectively, and are independent of the
system state at any time instant. Under this setting, the dynamical system Eq. (1)
is Markovian.

The optimal nonlinear filter recursively operates with a succession of prediction
and correction steps as summarized below. The reader is referred to Doucet et al.
(2001) for an extensive description of the filter. To simplify the notation, $\mathbf{y}_{1:k}$ is
defined as a shorthand for the set of all observations $\mathbf{y}_1, \dots, \mathbf{y}_k$ up to and including
time t_k . Let $p_k^f(\cdot | \mathbf{y}_{1:k-1})$ be the conditional (predictive) *pdf* of \mathbf{x}_k given $\mathbf{y}_{1:k-1}$ and
 $p_k^a(\cdot | \mathbf{y}_{1:k})$ be the conditional (analysis) *pdf* of \mathbf{x}_k given $\mathbf{y}_{1:k}$, both determined at
time t_k . The filter steps are described as follows.

- Prediction step: Given the analysis $pdf\ p_{k-1}^a(\cdot | \mathbf{y}_{1:k-1})$ at time t_{k-1} , the predictive $pdf\ p_k^f(\cdot | \mathbf{y}_{1:k-1})$ is obtained by integrating $p_{k-1}^a(\cdot | \mathbf{y}_{1:k-1})$ with the model (1) to the time of the next available observation t_k . Under the assumptions made on the model noise $\boldsymbol{\eta}_k$, the likelihood function for the state vector \mathbf{x}_{k-1} to transit to \mathbf{x}_k at the next time instant is described by the Gaussian $pdf\ N(\mathbf{x}_k : \mathbf{M}_k(\mathbf{x}_{k-1}), \mathbf{Q}_k)$, where $N(\mathbf{x} : \mu, \boldsymbol{\Sigma})$ denotes the Gaussian pdf with mean μ and covariance $\boldsymbol{\Sigma}$. Thus,

$$p_k^f(\mathbf{x}_k | \mathbf{y}_{1:k-1}) = \int_{\mathbb{R}^n} N(\mathbf{x}_k : \mathbf{M}_k(\mathbf{x}_{k-1}), \mathbf{Q}_k) p_{k-1}^a(\mathbf{x}_{k-1} | \mathbf{y}_{1:k-1}) d\mathbf{x}_{k-1}. \quad (3)$$

- Correction step: After a new observation \mathbf{y}_k has been made, the analysis $pdf\ p_k^a(\cdot | \mathbf{y}_{1:k})$ at time t_k is updated from $p_k^f(\cdot | \mathbf{y}_{1:k-1})$ using Bayes' rule, i.e.,

$$p_k^a(\mathbf{x}_k | \mathbf{y}_{1:k}) = \frac{1}{b_k} p_k^f(\mathbf{x}_k | \mathbf{y}_{1:k-1}) N(\mathbf{y}_k : \mathbf{H}_k(\mathbf{x}_k), \mathbf{R}_k). \quad (4)$$

The analysis pdf is therefore obtained by multiplying the predictive pdf by the observation likelihood function $N(\mathbf{y}_k : \mathbf{H}_k(\mathbf{x}_k), \mathbf{R}_k)$, and then being normalized by $b_k = \int_{\mathbb{R}^n} p_k^f(\mathbf{x}_k | \mathbf{y}_{1:k-1}) N(\mathbf{y}_k : \mathbf{H}_k(\mathbf{x}_k), \mathbf{R}_k) d\mathbf{x}_k$.

While the expressions of the state pdf s can be obtained conceptually, determining the exact values of them at each point of the state space is practically infeasible in high dimensional systems (Doucet et al., 2001). For instance, the determination of the predictive pdf requires the evaluation of the model $\mathbf{M}_k(\mathbf{x})$ for a prohibitively large number of \mathbf{x} , given that one single evaluation might already be computationally very expensive in realistic atmospheric and oceanic applications.

3 The Particle Ensemble Kalman Filter

3.1 Particle Kalman Filtering and Its Ensemble Implementation

Given N independent samples $\mathbf{x}^1, \dots, \mathbf{x}^N$ from a (multivariate) density p , an estimator \hat{p} of p can be obtained by the kernel density estimation method (Silverman, 1986), in the form of a mixture of N Gaussian *pdfs*:

$$\hat{p}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N N(\mathbf{x} : \mathbf{x}^i, \mathbf{P}), \quad (5)$$

where \mathbf{P} is a positive definite matrix. Inspired from this estimator, the particle Kalman filter (PKF) approximates the conditional state *pdfs* in the optimal nonlinear filter by mixtures of N Gaussian densities of the form

$$p_k^s(\mathbf{x}_k | \mathbf{y}_{1:k}) = \sum_{i=1}^N w_k^i N(\mathbf{x}_k : \mathbf{x}_k^{s,i}, \mathbf{P}_k^{s,i}). \quad (6)$$

The subscript s replaces a at the analysis time and f at the prediction time. The parameters of the mixture are the weights w_k^i , the centers of the distributions $\mathbf{x}_k^{s,i}$, and the covariance matrices $\mathbf{P}_k^{s,i}$. In particular, if $N = 1$, $p_k^s(\mathbf{x}_k | \mathbf{y}_{1:k})$ reduces to a single Gaussian *pdf*, so that the PKF reduces to the Kalman filter (KF) or its variants trivially (a non-trivial simplification will also be discussed below). Consequently, the KF and its variants can be considered special cases of the PKF.

Two special cases of Eq. (6) may be of particular interest. In the first case, $\mathbf{P}_k^{s,i} \rightarrow \mathbf{0}$, such that the Gaussian *pdfs* $N(\mathbf{x}_k : \mathbf{x}_k^{s,i}, \mathbf{P}_k^{s,i})$ tend to a set of Dirac functions $\delta(\mathbf{x}_k^{s,i})$, with the mass points at $\mathbf{x}_k^{s,i}$. In this case, the Gaussian mixture Eq. (6) reduces to the Monte Carlo approximation used in the particle filter (Doucet et al., 2001). In the second case, all Gaussian *pdfs* $N(\mathbf{x}_k : \mathbf{x}_k^{s,i}, \mathbf{P}_k^{s,i})$ have (almost) identical centers and covariances, such that the Gaussian mixture Eq. (6) tends to a (single) Gaussian approximation, an assumption often used in various nonlinear Kalman filters (including the EnKF). In this sense, the PKF can be considered as a filter

in between the Kalman filter and the particle filter (Hoteit et al., 2008; Luo et al., 2010).

The main procedures of the PKF are summarized as follows. Without loss of generality, suppose that at time instant $k - 1$, the analysis *pdf*, after a re-sampling step, is given by $\tilde{p}_{k-1}(\mathbf{x}_{k-1} \mid \mathbf{y}_{1:k-1}) = \sum_{i=1}^N \tilde{w}_{k-1}^i N(\mathbf{x}_{k-1} : \theta_{k-1}^i, \mathbf{\Phi}_{k-1}^i)$. Then by applying Eq. (3) at the prediction step, one obtains the background *pdf*, in terms of a new MON

$$p_k^f(\mathbf{x}_k \mid \mathbf{y}_{1:k-1}) \approx \sum_{i=1}^N \tilde{w}_{k-1}^i N(\mathbf{x}_k : \hat{\mathbf{x}}_k^{f,i}, \hat{\mathbf{P}}_k^{f,i}), \quad (7)$$

where $\hat{\mathbf{x}}_k^{f,i}$ and $\hat{\mathbf{P}}_k^{f,i}$ are the propagations of the mean θ_{k-1}^i and the covariance $\mathbf{\Phi}_{k-1}^i$ of the Gaussian component $N(\mathbf{x}_{k-1} : \theta_{k-1}^i, \mathbf{\Phi}_{k-1}^i)$ through the system model Eq. (1), respectively.

Given an incoming observation \mathbf{y}_k , one applies Eq. (4) to update $p_k^f(\mathbf{x} \mid \mathbf{y}_{1:k-1})$ to the analysis *pdf*, also in the form of an MON

$$p_k^a(\mathbf{x}_k \mid \mathbf{y}_{1:k}) = \sum_{i=1}^N w_k^i N(\mathbf{x}_k : \hat{\mathbf{x}}_k^{a,i}, \hat{\mathbf{P}}_k^{a,i}), \quad (8)$$

where $\hat{\mathbf{x}}_k^{a,i}$ and $\hat{\mathbf{P}}_k^{a,i}$ are updated from $\hat{\mathbf{x}}_k^{f,i}$ and $\hat{\mathbf{P}}_k^{f,i}$ through the Kalman filter or its variants, and the new weights

$$w_k^i = \frac{\tilde{w}_{k-1}^i N(\mathbf{y}_k : \mathbf{H}_k(\hat{\mathbf{x}}_k^{f,i}), \mathbf{\Sigma}_k^i)}{\sum_{j=1}^N \tilde{w}_{k-1}^j N(\mathbf{y}_k : \mathbf{H}_k(\hat{\mathbf{x}}_k^{f,j}), \mathbf{\Sigma}_k^j)}, \quad (9)$$

where $\mathbf{\Sigma}_k^i$ is the innovation matrix. If evaluated through the extended Kalman filter, $\mathbf{\Sigma}_k^i = \mathbf{H}_k^i \hat{\mathbf{P}}_k^{f,i} (\mathbf{H}_k^i)^T + \mathbf{R}_k$, with \mathbf{H}_k^i being the gradient of \mathbf{H}_k evaluated at $\hat{\mathbf{x}}_k^{f,i}$. Alternatively, if evaluated in the context of the EnKF, $\mathbf{\Sigma}_k^i$ can be expressed as the covariance of the projected background ensemble onto the observation space plus the observation covariance \mathbf{R}_k (Evensen, 1994; Whitaker and Hamill, 2002). Finally, a re-sampling step can be introduced to improve the performance of the PKF (Hoteit et al., 2008; Luo et al., 2010), so that the analysis *pdf* becomes $\tilde{p}_k(\mathbf{x}_k \mid \mathbf{y}_{1:k}) = \sum_{i=1}^N \tilde{w}_k^i N(\mathbf{x}_k : \theta_k^i, \mathbf{\Phi}_k^i)$. Such a re-sampling algorithm is presented in the next section.

The PKF correction step can be interpreted as composed of two types of corrections: a *Kalman-type correction* used to update $\hat{\mathbf{x}}_k^{f,i}$ and $\hat{\mathbf{P}}_k^{f,i}$ to $\hat{\mathbf{x}}_k^{a,i}$ and $\hat{\mathbf{P}}_k^{a,i}$, and a *particle-type correction* used to update the weights \tilde{w}_{k-1}^i to w_k^i . In the PKF, the Kalman correction reduces the risk of weights collapse by allocating the estimates $\hat{\mathbf{x}}_k^{f,i}$ (whose projections onto the observation space) far away from the observation \mathbf{y}_k relatively more weights than in the particle filter (Hoteit et al., 2008; Van Leeuwen, 2009). Indeed, Eq. (9) has the same form as in the PF (Doucet et al., 2001), but uses the innovation matrices Σ_k^i to normalize the model-data misfit, rather than \mathbf{R}_k . As Σ_k^i are always greater than \mathbf{R}_k , the estimates that are close to the observation will receive relatively less weights than in the PF, while those far from the observation will receive relatively more weights. This means that the support of the local predictive *pdf* and the observation likelihood function will be more coherent than in the PF. Re-sampling will therefore be needed less often, so that Monte Carlo fluctuations are reduced.

The main issue with the PKF is the prohibitive computational burden associated with running an ensemble of KFs, knowing that running a Kalman filter (KF) or an extended KF in high dimensional systems is already a challenge. To reduce computational cost, we use an ensemble of EnKFs, rather than the KF or the extended KF, to construct the PKF. We refer to this approach as the Particle Ensemble Kalman Filter (PEnKF). In the PEnKF, the (analysis) ensembles representing the Gaussian components are propagated forward in time to obtain a set of background ensembles at the next assimilation cycle. Then for each background ensemble, a stochastic or deterministic EnKF is used to update the background ensemble to its analysis counterpart. This amounts to simultaneously running a weighted ensemble of EnKFs, and the final state estimate is the weighted average of all the EnKFs solutions.

3.2 A Re-sampling Algorithm

We adopt a re-sampling algorithm that combines those in Hoteit et al. (2008); Luo et al. (2010); Pham (2001). The main idea is as follows: Given a MON, we first employ an information-theoretic criterion used in Hoteit et al. (2008) and Pham (2001) to check if it needs to conduct re-sampling. If there is such a need, we then re-approximate the MON by a new MON, based on the criterion that the mean and covariance of the new MON match those of the original MON as far as possible Luo et al. (2010).

More concretely, let $p(\mathbf{x})$ be the *pdf* of the n -dimensional random vector \mathbf{x} , expressed in terms of an MON with N Gaussian *pdfs* so that

$$p(\mathbf{x}) = \sum_{i=1}^N w_i N(\mathbf{x} : \mu_i, \Sigma_i) , \quad (10)$$

where w_i are the set of normalized weights of the Gaussian *pdfs* $N(\mathbf{x} : \mu_i, \Sigma_i)$ with mean μ_i and covariance Σ_i , satisfying $w_i \geq 0$ for $i = 1, \dots, N$ and $\sum_{i=1}^N w_i = 1$. To decide whether to conduct re-sampling or not, the entropy E_w of the weights w_i is computed, which reads (Hoteit et al., 2008; Pham, 2001)

$$E_w = - \sum_{i=1}^N w_i \log w_i . \quad (11)$$

Ideally, when the distribution of the weights w_i is uniform, which yields the maximum weight entropy $E_w^u = \log N$, there is no need to conduct re-sampling. Thus, as a criterion, if E_w is within a certain distance d to E_w^u , i.e.,

$$E_w^u - E_w = \log N + \sum_{i=1}^N w_i \log w_i \leq d , \quad (12)$$

where d is a user-defined threshold, then we choose not to conduct re-sampling. In this work we set the threshold $d = 0.25$ following Hoteit et al. (2008).

In case that there is a need to conduct re-sampling, we follow the procedure similar to that in Luo et al. (2010). Here the idea is to treat re-sampling as a *pdf* approximation problem, in which we seek a new MON

$$\tilde{p}(\mathbf{x}) = \frac{1}{q} \sum_{i=1}^q N(\mathbf{x} : \theta_i, \Phi_i) , \quad (13)$$

241 with q equally weighted Gaussian *pdfs*, to approximate the original $p(\mathbf{x})$ in Eq. (10).
 242 In approximation, we require that the mean and covariance of $\tilde{p}(\mathbf{x})$ be as close as
 243 possible to those of $p(\mathbf{x})$. To this end, we need to choose proper values of θ_i and Φ_i
 244 in order to achieve this objective.

The means and covariances of $p(\mathbf{x})$ and $\tilde{p}(\mathbf{x})$, denoted by $\bar{\mathbf{x}}$ and $\bar{\mathbf{P}}$, and $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{P}}$, respectively, are given by

$$\bar{\mathbf{x}} = \sum_{i=1}^N w_i \mu_i, \text{ and } \bar{\mathbf{P}} = \sum_{s=1}^N w_s \left(\Sigma_s + (\mu_s - \bar{\mathbf{x}})(\mu_s - \bar{\mathbf{x}})^T \right), \quad (14a)$$

$$\tilde{\mathbf{x}} = \frac{1}{q} \sum_{i=1}^q \theta_i, \text{ and } \tilde{\mathbf{P}} = \frac{1}{q} \sum_{i=1}^q \left(\Phi_i + (\theta_i - \tilde{\mathbf{x}})(\theta_i - \tilde{\mathbf{x}})^T \right). \quad (14b)$$

245 Thus our objective is equivalent to balancing the above equation such that

$$\tilde{\mathbf{x}} = \bar{\mathbf{x}}, \text{ and } \tilde{\mathbf{P}} \approx \bar{\mathbf{P}}. \quad (15)$$

246 In the trivial case with $q = N = 1$, Eq. (15) can be satisfied by letting $\theta_1 = \mu_1$ and
 247 $\Phi_1 = \Sigma_1$, and the PEnKF reduces to an EnKF. In non-trivial cases, for simplicity
 248 in solving Eq. (15) and reducing computational cost (as to be shown later), one may
 249 choose the covariances Φ_i to be constant, say $\Phi_i = \Phi$, for $i = 1, \dots, q$, so that

$$\frac{1}{q} \sum_{i=1}^q \theta_i = \bar{\mathbf{x}}, \text{ and } \Phi + \frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}})(\theta_i - \bar{\mathbf{x}})^T \approx \bar{\mathbf{P}}. \quad (16)$$

250 When an EnKF is used to construct the PKF, one needs to represent the solution
 251 of Eq. (16) in terms of some ensembles $\{\mathbf{X}_{en}^i, i = 1, \dots, q\}$, where \mathbf{X}_{en}^i is a matrix
 252 containing the (analysis) ensemble of the i th Gaussian component in Eq. (13), with
 253 mean θ_i and covariance Φ . For simplicity, we assume that \mathbf{X}_{en}^i are all of dimension
 254 $n \times m$, with the ensemble size m for each i . Similar results can be easily obtained in
 255 the case with non-uniform ensemble sizes.

256 We then define a constant c , called *fraction coefficient* hereafter, which satisfies
 257 that $0 \leq c \leq 1$. We let $\Phi \approx c^2 \bar{\mathbf{P}}$, so that Eq. (16) is reduced to

$$\frac{1}{q} \sum_{i=1}^q \theta_i = \bar{\mathbf{x}}, \text{ and } \frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}})(\theta_i - \bar{\mathbf{x}})^T \approx (1 - c^2) \bar{\mathbf{P}}. \quad (17)$$

In other words, the centers $\{\theta_i, i = 1, \dots, q\}$ can be generated as a set of state vectors whose sample mean and covariance are $\bar{\mathbf{x}}$ and $(1 - c^2)\bar{\mathbf{P}}$, respectively. After obtaining θ_i , one can generate the corresponding ensembles \mathbf{X}_{en}^i , with the sample means and covariances being θ_i and $\mathbf{\Phi} \approx c^2\bar{\mathbf{P}}$, respectively. How θ_i and \mathbf{X}_{en}^i can be generated is discussed with more details in the support material.

From the above discussion, we see that c is a coefficient that decides how to divide $\bar{\mathbf{P}}$ among $\mathbf{\Phi}$ and $\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}})(\theta_i - \bar{\mathbf{x}})^T$, so that the constraints in Eq. (16) are satisfied. When $c \rightarrow 0$, we have $\mathbf{\Phi} \rightarrow \mathbf{0}$ so that $\tilde{p}(\mathbf{x})$ in Eq. (13) approaches the Monte Carlo approximation in the particle filter, with the mass points equal to θ_i . On the other hand, when $c \rightarrow 1$, we have $\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}})(\theta_i - \bar{\mathbf{x}})^T \rightarrow \mathbf{0}$, so that all θ_i approach $\bar{\mathbf{x}}$ and $\mathbf{\Phi}$ approaches $\bar{\mathbf{P}}$. As a result, $\tilde{p}(\mathbf{x})$ in Eq. (13) approaches the Gaussian *pdf* $N(\mathbf{x} : \bar{\mathbf{x}}, \bar{\mathbf{P}})$, which is essentially the assumption used in the EnKF. In this sense, when equipped with the re-sampling algorithm, the PEnKF is a filter in between the particle filter and the EnKF, with an adjustable parameter c that influences its behavior.

We note that, when $c \rightarrow 0$, under the constraint of matching the first two moments, our re-sampling scheme is very close to the posterior Gaussian re-sampling strategy used in the Gaussian particle filter (Kotecha and Djurić, 2003; Xiong et al., 2006), in which one generates particles from a Gaussian distribution with mean and covariance equal to those of the posterior *pdf* of the system states. As a result, there is no guarantee that higher order moments of the new MON match those of the original MON in our re-sampling scheme. If matching higher-order moments is a concern, one may adopt alternative criteria, for instance, the one that aims to minimize the distance (in certain metric) between the new MON and the original one, so that the re-sampling procedure is recast as an optimization problem, in which one aims to choose appropriate parameters, i.e., means and covariances of the new MON, that satisfy the chosen criterion as far as possible. In principle, this type of parameter estimation problem may be solved by the expectation-maximization (EM) algorithm

(Redner and Walker, 1984; Smith, 2007). But in practice, it is often computationally very intensive in doing so, due to the slow convergence rate of the EM algorithm and the high dimensionality of the parameter space in constructing the new MON. Therefore we do not consider this type of more sophisticated re-sampling strategy in this study.

For the purpose of pdf re-approximation, it is clear that the MON is not the only choice. A few alternatives are developed in the context of kernel density estimation (KDE) (Silverman, 1986), and in principle all of them can be applied for pdf re-approximation. For instance, KDE is adopted at the re-sampling step in the regularized particle filter (RPF) (Musso et al., 2001; Stavropoulos and Titterton, 2001) to construct a continuous pdf with respect the particles before re-sampling, and to draw a number of new particles from the continuous pdf afterwards. In this regard, the PEnKF is similar to the RPF, especially if the Gaussian kernel is adopted in the RPF for density estimation. However, there also exist differences. We list some of them as follows.

- The RPF first constructs a continuous pdf, and then draws a number of new particles with equal weights from the resulting pdf. In contrast, the PEnKF aims to directly approximate a MON by a new MON with equal weights.
- In the RPF, various kernels can be adopted for the purpose of constructing the continuous pdf. However, in the PEnKF, we are confined to use the MON, since we aim to build the PEnKF consisting of a set of parallel EnKFs.
- The pdf re-approximation criterion used in the PEnKF only captures the first two moments of the underlying pdf. In contrast, KDE used in the RPF in principle can yield a very good pdf estimate, provided that there are sufficient particles. In certain circumstances, though, the number of required particles may also suffer from the “curse-of-dimensionality” (Silverman, 1986, ch. 4).

3.3 Outline of the PEnKF Algorithm

To facilitate the comprehension of the PEnKF, here we provide an outline of the main steps of its algorithm. To avoid distraction, we will discuss the initialization of the PEnKF in the next section. Throughout this paper, we assume that the number q of Gaussian components at the re-sampling step and the number N of Gaussian components at the prediction and correction steps are time invariant. This implies the choice $q = N$.

Without loss of generality, we also assume that at time instant $k-1$, the posterior pdf $p_{k-1}^a(\mathbf{x}_{k-1} \mid \mathbf{y}_{1:k-1})$ is re-approximated, through the re-sampling step, by a mixture model

$$\tilde{p}_{k-1}(\mathbf{x}_{k-1} \mid \mathbf{y}_{1:k-1}) = \sum_{i=1}^q \tilde{w}_{k-1}^i N(\mathbf{x}_{k-1} : \theta_{k-1,i}, \mathbf{\Phi}_{k-1}) .$$

Moreover, the re-approximated analysis ensembles $\{\mathbf{X}_{approx}^{k-1,i}, i = 1, \dots, q\}$ representing the Gaussian components $N(\mathbf{x}_{k-1} : \theta_{k-1,i}, \mathbf{\Phi}_{k-1})$ are also generated. The procedures at the next assimilation cycle are outlined as follows.

- Prediction step: For $i = 1, \dots, q$, propagate the ensembles $\mathbf{X}_{approx}^{k-1,i}$ forward through Eq. (1) to obtain the corresponding background ensembles $\mathbf{X}_{bg}^{k,i}$ at instant k . Accordingly, the background pdf becomes

$$p_k^b(\mathbf{x}_k \mid \mathbf{y}_{1:k-1}) = \sum_{i=1}^q \tilde{w}_{k-1}^i N(\mathbf{x}_k : \hat{\mathbf{x}}_{k,i}^b, \hat{\mathbf{P}}_{k,i}^b) ,$$

with $\hat{\mathbf{x}}_{k,i}^b$ and $\hat{\mathbf{P}}_{k,i}^b$ being the sample mean and covariance of the ensemble $\mathbf{X}_{bg}^{k,i}$, respectively.

- Correction step: With an incoming observation \mathbf{y}_k , for each background ensemble $\mathbf{X}_{bg}^{k,i}$, $i = 1, \dots, q$, apply an EnKF to obtain the analysis mean $\hat{\mathbf{x}}_{k,i}^a$ and the analysis ensemble $\mathbf{X}_{ana}^{k,i}$. During the correction, covariance inflation and localization (cf. § 4.2.2) can be conducted on the EnKF. In addition, update the associated weights \tilde{w}_{k-1}^i to w_k^i according to Eq (9). After the corrections, the

analysis *pdf* becomes

$$p_k^a(\mathbf{x}_k \mid \mathbf{y}_{1:k}) = \sum_{i=1}^q w_k^i N\left(\mathbf{x}_k : \hat{\mathbf{x}}_{k,i}^a, \hat{\mathbf{P}}_{k,i}^a\right),$$

where w_k^i are computed according to Eq. (9) in the context of the EnKF, and $\hat{\mathbf{P}}_{k,i}^a$ are the sample covariances of $\mathbf{X}_{ana}^{k,i}$.

- Re-sampling step: Use the criterion in (12) to determine whether to conduct re-sampling or not.

(1) If there is no need for re-sampling, then assign $\tilde{p}_k(\mathbf{x}_k \mid \mathbf{y}_{1:k}) = p_k^a(\mathbf{x}_k \mid \mathbf{y}_{1:k})$,

and $\mathbf{X}_{approx}^{k,i} = \mathbf{X}_{ana}^{k,i}$ for $i = 1, \dots, q$;

(2) Otherwise, $\tilde{p}_k(\mathbf{x}_k \mid \mathbf{y}_{1:k}) = \frac{1}{q} \sum_{i=1}^q N(\mathbf{x}_k : \theta_{k,i}, \mathbf{\Phi}_k)$, where parameters $\theta_{k,i}$

and $\mathbf{\Phi}_k$ are computed following the method in § 3.2, and the associated

weights become $1/q$. The ensembles $\mathbf{X}_{approx}^{k,i}$ are produced accordingly.

4 Numerical Experiments

4.1 Experiment Design

In the present work, we focus on two different implementations of the PEnKF: the first is based on the stochastic EnKF (SEnKF) of Evensen (1994) and the second based on the ensemble transform Kalman filter (ETKF) of Bishop et al. (2001). These two implementations are referred to as the PSEnKF and the PETKF, respectively.

The strongly nonlinear 40-dimensional system model due to Lorenz and Emanuel (1998) (LE98 model hereafter) was chosen as the testbed to evaluate and study the performance of these two filters. This model mimics the time-evolution of a scalar atmospheric quantity. It is governed by the following set of equations:

$$\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})x_{i-1} - x_i + 8, \quad i = 1, \dots, 40, \quad (18)$$

where the nonlinear quadratic terms simulate advection and the linear term represents dissipation. Boundary conditions are cyclic, i.e. we define $x_{-1} = x_{39}$, $x_0 = x_{40}$, and $x_{41} = x_1$. The model was numerically integrated using the Runge-Kutta fourth order scheme from time $t = 0$ to $t = 35$ with a constant time step $\Delta t = 0.05$ (which corresponds to 6 hours in real time). To eliminate the impact of transition states, the model trajectory between times $t = 0$ and $t = 25$ was discarded. The assimilation experiments were carried out during the period $t = 25.05$ to $t = 35$ where the model trajectory was considered to be the 'truth'. Reference states were then sampled from the true trajectory and a filter performance is evaluated by how well it is able to estimate the reference states using a perturbed model and assimilating a set of (perturbed) observations that was extracted from the reference states.

In this work we consider two scenarios: one with a linear observation operator and the other with a nonlinear operator. The concrete forms of these two observational operators will be given in the relevant sections below.

The time-averaged root mean squared error (rmse for short) is used to evaluate the performance of a filter. Given a set of n -dimensional state vectors $\{\mathbf{x}_k : \mathbf{x}_k = (x_{k,1}, \dots, x_{k,n})^T, k = 0, \dots, k_{max}\}$, with k_{max} being the maximum time index ($k_{max} = 199$ in our experiments), then the rmse \hat{e} is defined as

$$\hat{e} = \frac{1}{k_{max} + 1} \sum_{k=0}^{k_{max}} \sqrt{\frac{1}{n} \sum_{i=1}^n (\hat{x}_{k,i}^a - x_{k,i})^2}, \quad (19)$$

where $\hat{\mathbf{x}}_k^a = (\hat{x}_{k,1}^a, \dots, \hat{x}_{k,n}^a)^T$ is the analysis state of \mathbf{x}_k .

A possible problem in directly using \hat{e} as the performance measure is that \hat{e} itself may depend on some intrinsic parameters of the filters, for instance, the covariance inflation factor and localization length scale as to be discussed later. This may lead to inconsistent conclusions at different parameter values. To avoid this problem, we adopted the following strategy: we relate a filter's best possible performance to the minimum rmse \hat{e}_{min} , which is the minimum value of \hat{e} that the filter can achieve within the chosen ranges of the filter's intrinsic parameters. In performance comparison, if

the minimum rmse \hat{e}_{min}^A of filter A is less than the minimum rmse \hat{e}_{min}^B of filter B ,
 filter A is said to perform better than filter B .

4.2 Implementation Details

4.2.1 Filter Initialization

To initialize the PEnKF, we first estimate the mean and covariance of the LE98 model over some time interval following Hoteit et al. (2008). These statistics are then used to produce the $pdf\ p_0^f(\mathbf{x}_0)$ of the background at the first assimilation cycle as a MON.

Concretely, the LE98 model was first integrated for a long period (between $t = 0$ and $t = 1000$) starting from an initial state that has been drawn at random. The trajectory that falls between $t = 50.05$ and $t = 1000$ was used to estimate the mean $\hat{\mathbf{x}}_{ds}$ and covariance $\hat{\mathbf{P}}_{ds}$ of the dynamical system. To initialize $p_0^f(\mathbf{x}_0)$ as a mixture of N Gaussian distributions

$$p_0^f(\mathbf{x}_0) = \frac{1}{N} \sum_{i=1}^N N(\mathbf{x}_0 : \mathbf{x}_0^{f,i}, \mathbf{P}_{com}), \quad (20)$$

where $\mathbf{x}_0^{f,i}$ are the means, and \mathbf{P}_{com} the common covariance matrix of the Gaussian distributions in the mixture, we draw N samples $\mathbf{x}_0^{f,i}$ from the Gaussian distribution $N(\mathbf{x}_0 : \hat{\mathbf{x}}_{ds}, \hat{\mathbf{P}}_{ds})$, and set $\mathbf{P}_{com} = \hat{\mathbf{P}}_{ds}$. If $\hat{\mathbf{x}}_0^f = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_0^{f,i}$ denotes the sample mean of $\mathbf{x}_0^{f,i}$, then the covariance \mathbf{P}_0^f of $p_0^f(\mathbf{x}_0)$ is given by

$$\mathbf{P}_0^f = \hat{\mathbf{P}}_{ds} + \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_0^{f,i} - \hat{\mathbf{x}}_0^f)(\mathbf{x}_0^{f,i} - \hat{\mathbf{x}}_0^f)^T, \quad (21)$$

which is always larger than $\hat{\mathbf{P}}_{ds}$. The rationale behind this choice is not far from the covariance inflation technique (Anderson and Anderson, 1999; Whitaker and Hamill, 2002). In practice, a data assimilation system is often subject to various errors, such as poorly known model and observational errors, sampling errors, etc. In such circumstances, an inflated background covariance would allocate more weights to the incoming observation when updating the background to the analysis, making the filter more robust (Jazwinski, 1970; Simon, 2006).

4.2.2 Covariance Inflation and Localization

Covariance inflation (Anderson and Anderson, 1999; Whitaker and Hamill, 2002) and localization (Hamill et al., 2001) are two popular techniques that are used to improve the stability and performance of the EnKF (Hamill et al., 2009; Van Leeuwen, 2009), especially in the small ensemble scenario. In our experiments, these two techniques are implemented for each EnKF in the PEnKF.

More concretely, to introduce covariance inflation to the i th EnKF at instant k , we multiply the analysis covariance $\hat{\mathbf{P}}_{k,i}^a$ (before the re-sampling step) by a factor $(1 + \delta)^2$, where the scalar $\delta \geq 0$, called *covariance inflation factor*, is introduced as an intrinsic parameter of the EnKF. On the other hand, we follow the method in Hamill et al. (2001) to conduct covariance localization on the background covariance and its projection onto the observation space, with the tapering function (for smoothing out spuriously large values in covariance matrices) being the fifth order function defined in Eq. (4.10) of Gaspari and Cohn (1999). In doing so, another intrinsic scalar parameter $l_c > 0$, called *length scale* (Hamill et al., 2001), is introduced to the EnKF. Roughly speaking, l_c is a parameter that determines the critical distance beyond which the tapering function becomes zero.

4.3 Experiments Results with a Linear Observation Operator

In the first scenario, we let the (synthetic) observations be generated every day (4 model time steps) from the reference states using the following linear observation system

$$\mathbf{y}_k = (x_{k,1}, x_{k,3}, \dots, x_{k,39})^T + \mathbf{v}_k, \quad (22)$$

where only the odd state variables $x_{k,i}$ ($i = 1, 3, \dots, 39$) of the system state $\mathbf{x}_k \equiv (x_{k,1}, \dots, x_{k,40})^T$ at time index k are observed. The observation noise \mathbf{v}_k follows the 20-dimensional Gaussian distribution $N(\mathbf{v}_k : \mathbf{0}, \mathbf{I}_{20})$ with \mathbf{I}_{20} being the 20×20 identity

429 matrix.

430 4.3.1 Effect of the Number of Gaussian Distributions

431 In the first experiment we examine the effect of the number of Gaussian distributions
432 on the performance of the PSEnKF and the PETKF. The experiment settings are as
433 follows.

434 We initialize the pdf $p_0^f(\mathbf{x}_0)$ with N Gaussian *pdfs*. In our experiments we let N
435 take values between 1 and 60. Since it is costly to carry out the computation for
436 each integer in this interval, we choose to let N increase from 1 to 10, with an even
437 increment of 1 each time, and then increase it from 15 to 60, with a larger incre-
438 ment of 5 each time, as N becomes larger. For convenience, we denote this choice
439 by $N \in \{1 : 1 : 10, 15 : 5 : 60\}$, where the notation $v_{min} : v_{inc} : v_{max}$ represents a
440 set of values increasing from v_{min} to v_{max} , with an even increment of v_{inc} each time.
441 If there is a need to conduct re-sampling, we re-approximate the analysis MON by
442 a new MON with equal weights and with the same number of normal distributions.
443 In doing so, we introduce a new parameter, i.e., the fraction coefficient c defined in
444 § 3.2, to the PSEnKF/PETKF. To examine its effect on the performance of the
445 filter, we let $c \in \{0.05 : 0.1 : 0.95\}$. The ensemble size is set to $m = 20$ in each
446 SEnKF/ETKF, which is relatively small compared to the system dimension 40. In
447 this case, it is customary to conduct covariance inflation (Anderson and Anderson,
448 1999; Whitaker and Hamill, 2002) and localization (Hamill et al., 2001) to improve
449 the robustness and performance of the filters (Hamill et al., 2009; Van Leeuwen,
450 2009). The impacts of covariance inflation and localization on the performance of the
451 EnKF have been examined in many works, see, for example, Whitaker and Hamill
452 (2002). In our experiments we let the covariance inflation factor $\delta = 0.02$. We follow
453 the settings in Luo et al. (2010, § 7.2.3) to conduct covariance localization and choose
454 the length scale $l_c = 50$. To reduce statistical fluctuations, we repeat the experiments
455 for 20 times, each time with a randomly drawn initial background ensemble, but the

same true trajectory and the corresponding observations. The same repetition setting is adopted in all the other experiments.

In Fig. 1 we show the rms errors of both the PSEnKF and PETKF as functions of the fraction coefficient c and the number N of Gaussian *pdfs*. First, we examine how the rmse of the PSEnKF changes with c when N is fixed. In Fig. 1(a), if N is relatively small (say $N < 40$), the rmse tends to decrease as c increases. For larger N (say $N = 55$), the rmse of the filter exhibits the bell-shape behavior: at the beginning it increases when c grows from 0; after c becomes relatively large (say $c = 0.4$), further increasing c reduces the rmse instead. Next, we examine the behavior of the rmse of the PSEnKF with respect to N when c is fixed. When c is relatively small (say $c = 0.1$), the rmse exhibits the U-turn behavior: at the beginning it intends to decrease as N grows; after N becomes relatively large (say $N = 45$), further increasing N increases the rmse instead. When c is larger, say, $c = 0.6$, the rmse appears less sensitive to the change of N . However, for even larger values of c , say, $c = 0.9$, the rmse appears to monotonically decrease with N .

The behavior of the PETKF (cf. Fig. 1(b)) with respect to the changes of N and c is similar to that of the PSEnKF. Therefore we do not repeat its description here.

To examine the minimum rms errors \hat{e}_{min} of the PSEnKF and the PETKF within the tested values of c and N , we plot \hat{e}_{min} of both filters as functions of N in Fig. 2. The \hat{e}_{min} of both filters tends to decrease as the number N of Gaussian distributions increases, though there also exhibit certain local minima. The PSEnKF achieves its lowest \hat{e}_{min} at $N = 60$, while the PETKF at $N = 50$. As N grows, both the PSEnKF and the PETKF tend to have lower \hat{e}_{min} than their corresponding base filters, the SEnKF and the ETKF (corresponding to the PSEnKF and the PETKF with $N = 1$, as discussed in § 3.2), respectively. This confirms the benefit of accuracy improvement by using the PEnKF instead of an EnKF. A comparison between the PSEnKF and the PETKF shows that the PETKF performs better than the PSEnKF when the number N of Gaussian distributions is relatively small (say, $N \leq 7$). However, as

484 N becomes larger, the PSEnKF outperforms its ETKF-based counterpart instead.

485 Similar phenomena can also be observed in other experiments, as to be shown later.

486 4.3.2 Effect of the Ensemble Size

487 In the second experiment we examine the effect of the ensemble size of each SEnKF/ETKF
488 in the PEnKF, on the performance of the PSEnKF/PETKF. For reference, we also
489 examine the performance of the SEnKF and the ETKF under various ensemble sizes.

490 The experiment settings are as follows. For the PSEnKF and the PETKF, we let the
491 ensemble size m of each EnKF take values from the set $\{20, 40, 80, 100, 200, 400, 800, 1000\}$.
492 For a single SEnKF/ETKF, we let $m \in \{20, 40, 60, 80, 100, 200, 400, 600, 800, 1000\}$,
493 with two more values at 60 and 600.

494 In the PSEnKF and the PETKF, we also vary the fraction coefficient c such that
495 $c \in \{0.05 : 0.1 : 0.95\}$. We fix the number N of Gaussian *pdfs*, i.e., the number of
496 ensemble filters, to be 3. To conduct covariance inflation, we let the inflation factor
497 $\delta = 0.02$. We choose to conduct covariance localization, and set the length scale
498 $l_c = 50$, only if the ensemble size m is not larger than the dimension 40 of the LE98
499 model. No covariance localization was conducted if $m > 40$. Our experience shows
500 that, for $m > 40$, the benefit of conducting localization is not significant even if the
501 length scale l_c is properly chosen, while an improper value of l_c is more likely to
502 deteriorate the filter performance. To reduce statistical fluctuations, the experiments
503 are again repeated for 20 times.

504 In Fig. 3 we show the rms errors of the SEnKF and the ETKF as functions of
505 the ensemble size m . The rmse of the ETKF exhibits a U-turn behavior. The rmse
506 of the ETKF monotonically decreases as long as $m < 100$. Beyond that, the rmse
507 monotonically increases instead as m increases. On the other hand, the SEnKF
508 exhibits a different behavior. Its rmse decreases for $m \leq 200$, and then reaches a
509 plateau where the rmse remains almost unchanged as m further increases.

510 Fig. 4 plots the rms errors of the PSEnKF and the PETKF as functions of the

fraction coefficient c , and the ensemble size m in the SEnKF and the ETKF used to construct the corresponding PEnKFs. The rms errors, as functions of the ensemble size m (with fixed c), are consistent with our observations in Fig. 3. On the other hand, for both PEnKFs, their rms errors tend to decrease as the fraction coefficient c increases.

Per analogy to the first experiment, Fig. 5 plots the minimum rms errors \hat{e}_{min} of the PSenKF and the PETKF within the tested fraction coefficient c and the ensemble size m . A comparison between Figs. 5 and 3 shows that, the minimum rms errors \hat{e}_{min} of the PEnKFs behave very similarly to the rms errors of their corresponding EnKFs in Fig. 3. Moreover, the values of \hat{e}_{min} in Fig. 5 tends to be lower than the corresponding rms errors in Fig. 3, indicating the benefit of accuracy improvement in using the PEnKFs. Again, a comparison between the PSenKF and the PETKF shows that the PETKF performs better than the PSenKF when the ensemble size m is relatively small (say, $m \leq 40$). However, as m becomes larger, the PSenKF outperforms the PETKF instead.

4.4 Experiments Results with a Nonlinear Observation Operator

In the second scenario, we introduce nonlinearity to the observation system. To this end, we let the observations be generated by the following nonlinear process

$$\mathbf{y}_k = 0.05(x_{k,1}^2, \dots, x_{k,39}^2)^T + \mathbf{v}_k \quad (23)$$

for every 4 model time steps. In Eq. (23), again only the odd state variables $x_{k,i}$ ($i = 1, 3, \dots, 39$) of the system state $\mathbf{x}_k \equiv (x_{k,1}, \dots, x_{k,40})^T$ at time index k are observed. The observation noise \mathbf{v}_k also follows the 20-dimensional Gaussian distribution $N(\mathbf{v}_k : \mathbf{0}, \mathbf{I}_{20})$. We conduct the same experiments as those in the case of linear observation operator.

4.4.1 Effect of the Number of Gaussian Distributions

We first examine the effect of the number of Gaussian distributions. The experiment settings are the same as those in § 4.3.1. Concretely, For either the PSEnKF or the PETKF, the number of Gaussian distributions $N \in \{1 : 1 : 10, 15 : 5 : 60\}$, the fraction coefficient $c \in \{0.05 : 0.1 : 0.95\}$. For each individual SEnKF/ETKF in the PEnKF, the ensemble size $m = 20$, the covariance inflation factor $\delta = 0.02$ and the length scale $l_c = 50$ for covariance localization. As before, the experiments are repeated for 20 times to reduce statistical fluctuations.

Fig. 6 plots the rms errors of both the PSEnKF and the PETKF as functions of the fraction coefficient c and the number N of Gaussian *pdfs*. When c and N changes, both the PSEnKF and the PETKF behave very similar to their counterparts in the linear case. The rms errors of the filters tend to decrease as N increases, meaning that the PSEnKF/PETKF with $N > 1$ in general performs better than the stochastic EnKF /ETKF (corresponding to the case $N = 1$ in the PEnKF), consistent with the results obtained in the linear observer case.

We also examine the minimum rms errors \hat{e}_{min} of the PSEnKF and the PETKF within the tested values of c and N . Fig. 7 plots \hat{e}_{min} as functions of N . For the PSEnKF, the lowest \hat{e}_{min} is achieved at $N = 50$. And for the PETKF, its \hat{e}_{min} tends to decrease within the tested range of N , and achieves its minimum at $N = 60$. The PEnKF with more than one Gaussian distributions ($N > 1$) performs better than the corresponding EnKF ($N = 1$). In addition, a comparison between the PSEnKF and the PETKF shows again that the PETKF performs better than the PSEnKF when the number N of Gaussian distributions is relatively small, but tends to become worse as N increases.

A comparison between Figs. 2 and 7 shows that the rmse of a filter (e.g. the PSEnKF at $N = 2$) with a nonlinear observer sometimes may be lower than that of the same filter with a linear observer ¹. This seemingly counter-intuitive result

¹The result of comparison would also depend on the filter in use, its configuration, the system in

happens possibly because in such situations, the effect of sampling error due to the relatively small ensemble size dominates the effect of nonlinearity in the observation system. However, as the number N of Gaussian distributions increases, the effect of nonlinearity becomes more prominent so that the rmse with a nonlinear observer tends to be higher than that with a linear one. Similar phenomenon can also be found by comparing Figs. 3 and 5 with Figs. 8 and 10 (to be shown below), respectively, at different ensemble sizes.

4.4.2 Effect of the Ensemble Size

In the second experiment we examine the effect of the ensemble size in each ensemble filter on the performance of the corresponding PEnKF. For reference, we also examine the performance of the SEnKF and the ETKF under various ensemble sizes. The experiment settings are the same as those in § 4.3.2. In the PSEnKF and PETKF, we choose the fraction coefficient $c \in \{0.05 : 0.1 : 0.95\}$. We also choose the number of ensemble filters in each PEnKF to be 3. For each individual EnKF in the corresponding PEnKF, we let the ensemble size m take values from the set $\{20, 40, 80, 100, 200, 400, 800, 1000\}$, and for the experiments on the single EnKF, we let $m \in \{20, 40, 60, 80, 100, 200, 400, 600, 800, 1000\}$. To conduct covariance inflation and localization in each individual EnKF, we choose the inflation factor $\delta = 0.02$, and the length scale $l_c = 50$. As in § 4.3.2, covariance localization is conducted only if the ensemble size m is no larger than the dimension 40.

Fig. 8 shows the rms errors of the SEnKF and the ETKF as functions of the ensemble size m . For both filters, their rms errors decrease as the ensemble size m increases. The ETKF performs better than the SEnKF in the small sample scenario with $m = 20$. But as m increases, the SEnKF outperforms the ETKF instead. In particular, divergence in the ETKF occurs if $m > 400$, which did not happen in the linear observer case (cf. Fig. 3). On the other hand, the rmse of the SEnKF appears

assimilation, and so on, and therefore may change from case to case.

to reach a plateau for $m > 400$, similar to the linear observer case. Comparing Fig. 8 with Fig. 3, it is easy to see that, except for the stochastic EnKF at $m = 20$, the presence of nonlinearity in the observer deteriorates the performance of the ensemble filters.

Fig. 9 plots the rms errors of the PSEnKF and the PETKF as functions of the fraction coefficient c , and the ensemble size m in the corresponding SEnKF and the ETKF, respectively. In the PSEnKF (cf. Fig. 9(a)), the rmse tends to decrease as both c and m increases when the ensemble size $m \leq 800$. However, when $m > 800$, the impact of m on the filter performance is not significant, which is consistent with the results in Fig. 8. On the other hand, in the PETKF (cf. Fig. 9(b)), filter divergence occurs for $m > 200$, which is why we only report its rmse with $m \leq 200$ in Fig. 9(b), where the rmse of the PETKF appears to be a monotonically decreasing function of m and c .

In analogy to the first experiment, Fig. 10 plots the minimum rms errors \hat{e}_{min} of the PSEnKF and the PETKF within the tested fraction coefficient c and ensemble size m . One may observe that, similar to the SEnKF and the ETKF themselves, the \hat{e}_{min} of both the PSEnKF and the PETKF decrease as m increases. However, for the PETKF, divergence occurs if $m > 200$, rather than $m > 400$ as in Fig. 8, but overall its rmse is closer to that obtained in the PSEnKF. Meanwhile, a comparison between Fig. 8 and Fig. 10 shows that the PEnKFs perform better than the corresponding EnKFs. Also, a comparison between Fig. 5 and 10 shows that, except for the PSEnKF at $m = 20$, the nonlinearity in the observer again deteriorates the performance of the ensemble filters.

5 Discussion

This paper presented a discrete solution of the optimal nonlinear filter, called the particle Kalman filter (PKF), based on the Gaussian mixture representation of the state

pdf given the observations. The PKF solves the nonlinear Bayesian correction step by complementing the Kalman filter-like correction step of the particles with a particle filter-like correction step of the weights. The PKF simultaneously runs a weighted ensemble of the Kalman filters in parallel. This is far beyond our computing capabilities when dealing with computationally demanding systems, as the atmospheric and oceanic models. Therefore, to reduce computational cost, one may instead consider a low-rank parametrization of the Gaussian mixture covariance matrices of the state pdf s. An efficient way to do that is to resort to the ensemble Kalman filter (EnKF) and use an EnKF-like method to update each component of the Gaussian mixture pdf s. This amounts to running a weighted ensemble of the EnKFs. In this work, the PKF was implemented using the stochastic EnKF and a deterministic EnKF, the ensemble transform Kalman filter (ETKF). We call this type of implementation the particle ensemble Kalman filter (PEnKF).

The PEnKF sets a nonlinear Bayesian filtering framework that encompasses the EnKF methods as a special case. As in the EnKF, the Kalman correction in the PEnKF attenuates the degeneracy of the ensemble by allocating the ensemble members far away from the incoming observation relatively more weights than in the particle filter, so that the filter can operate with reasonable size ensembles. To further improve the performance of the PEnKF, we also introduced to the PEnKF a re-sampling step similar to that used in the regularized particle filter (Musso et al., 2001; Stavropoulos and Titterton, 2001).

The stochastic EnKF and ETKF-based PEnKFs, called the PSEnKF and the PETKF, respectively, were implemented and their performance was investigated with the strongly nonlinear Lorenz-96 model. These filters were tested with both linear and nonlinear observation operators. Experiments results suggest that the PSEnKF and the PETKF outperform their corresponding EnKFs. It was also found that the ETKF outperforms the stochastic EnKF for small size ensembles while the stochastic EnKF exhibits better performance for large size ensembles. We argued that this

happens because the EnKF endures less observational sampling errors when the ensemble size is large. Another reason would also be the better approximation of the PEnKF distributions provided by the stochastic EnKF compared to the ETKF. This was also true for their PEnKF counterparts. Overall, the conclusions from the numerical results obtained with the linear and nonlinear observation operators were not fundamentally different, except that in general better estimation accuracy was achieved with the linear observer when the sampling error is not the dominant factor. The results also suggest that the PEnKFs could more benefit from the use of more components in the mixture of normals (MON) and larger ensembles in the EnKFs in the nonlinear observations case.

Future work will focus on developing and testing new variants of the PEnKF that applies more efficient approximations, in term of computational cost, to update the mixture covariance matrices. Another direction for improvement would be also to work on localizing the correction step of the particle weights (Van Leeuwen, 2009). Our final goal is to develop a set of computationally feasible suboptimal PEnKFs that can outperform the EnKF methods at reasonable computational cost. As stated by Anderson (2003), developing filters in the context of the optimal nonlinear filtering problem, rather than starting from the Kalman filter, should lead to a more straightforward understanding of their capabilities.

The paper further discussed how the PEnKF can also be used as a general framework to simultaneously run several assimilation systems. We believe that this approach provides a framework to merge the solutions of different EnKFs, or to develop hybrid EnKF-variational methods. Work in this direction is under investigation.

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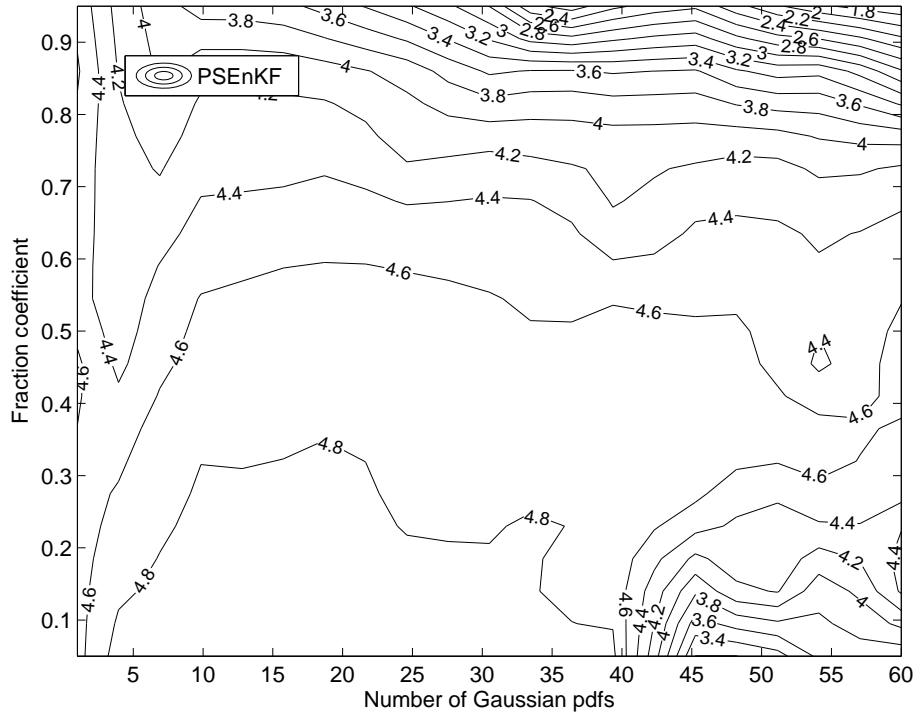
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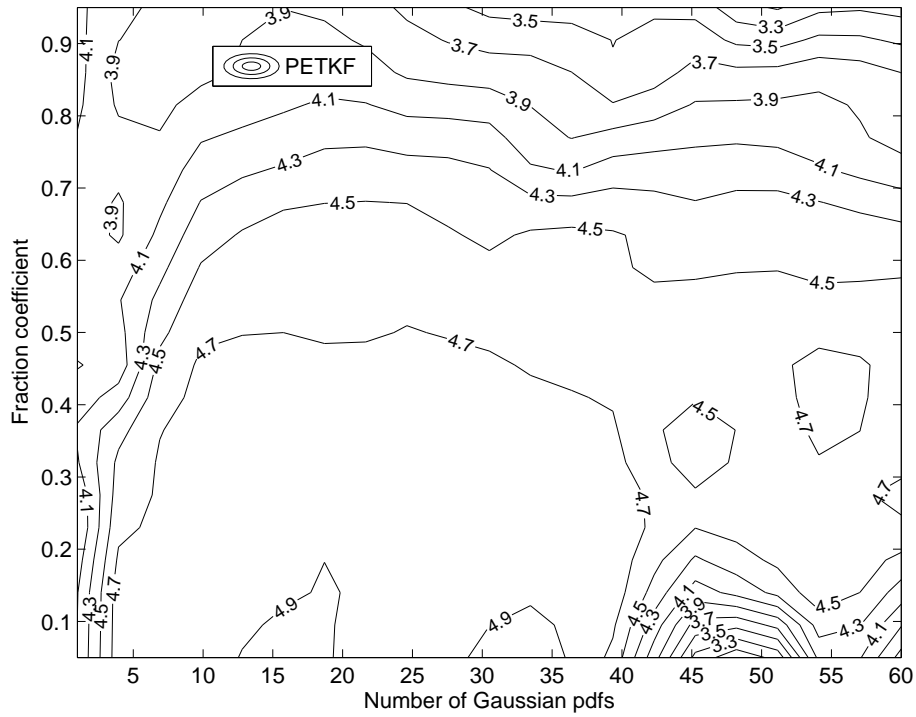
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(a) Stochastic EnKF-based PKF



(b) ETKF-based PKF

Figure 1: RMS errors (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed ensemble size of 20 in each ensemble filter) as the functions of the fraction coefficient and the number of Gaussian it pdfs in the MON.

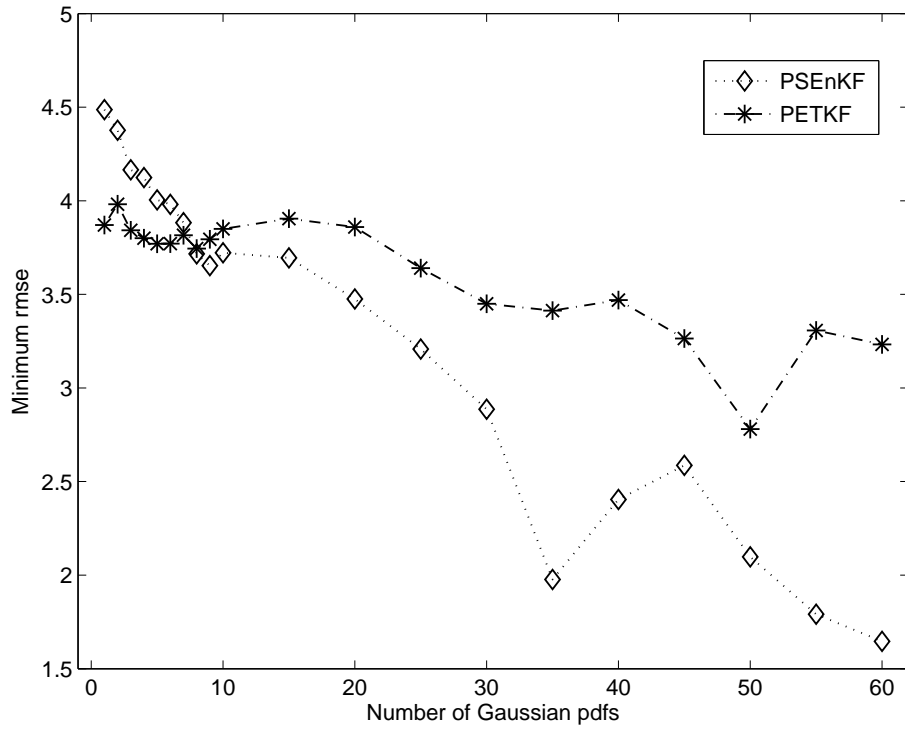


Figure 2: Minimum rms errors \hat{e}_{min} (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed ensemble size of 20 in each ensemble filter) as the function of the number of Gaussian *pdfs* in the MON.

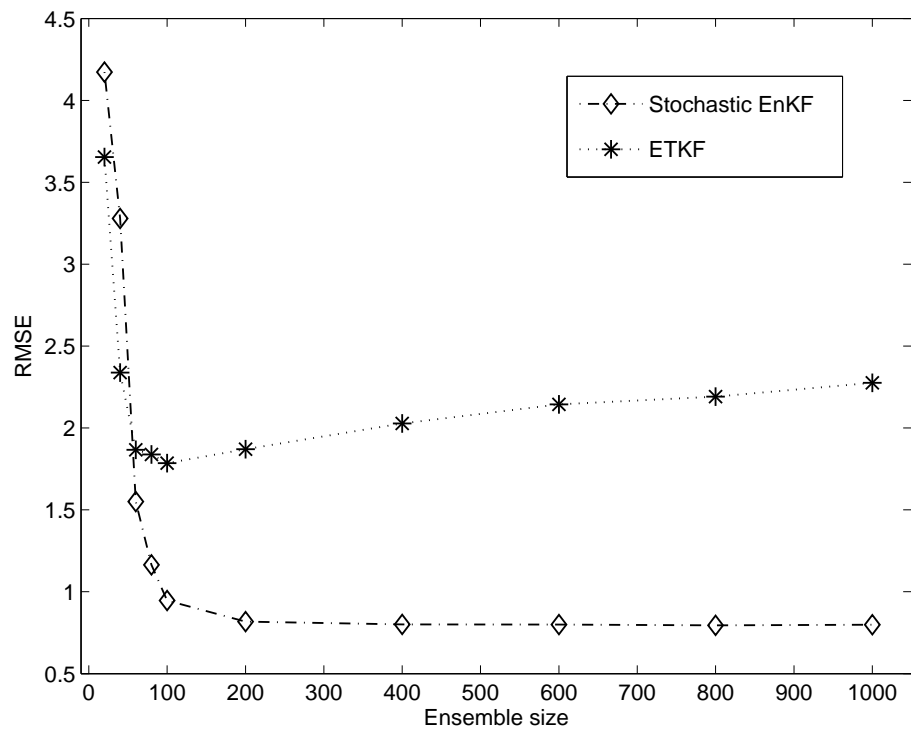
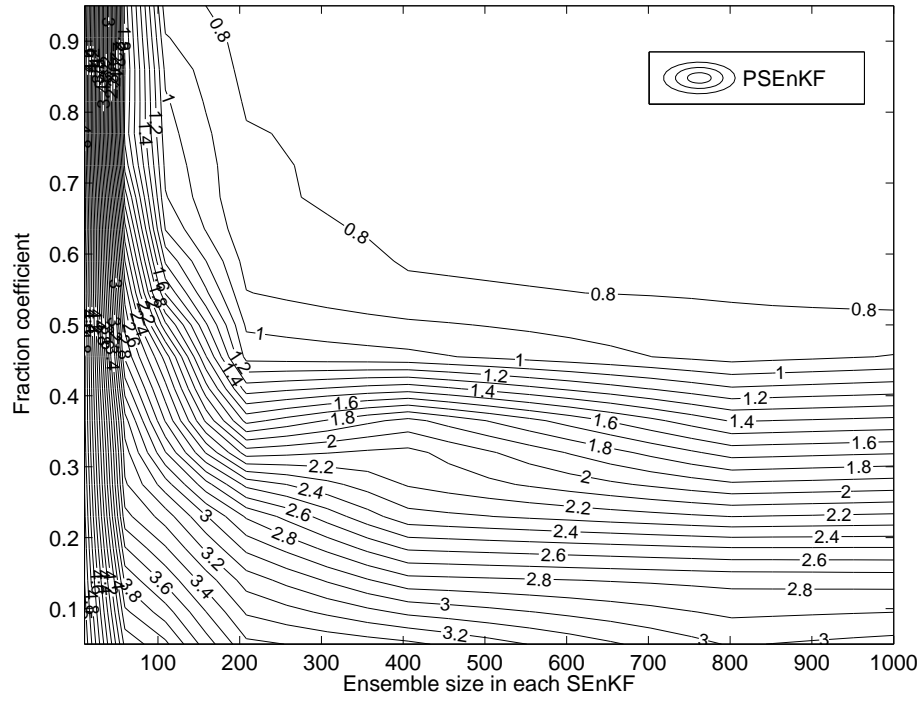
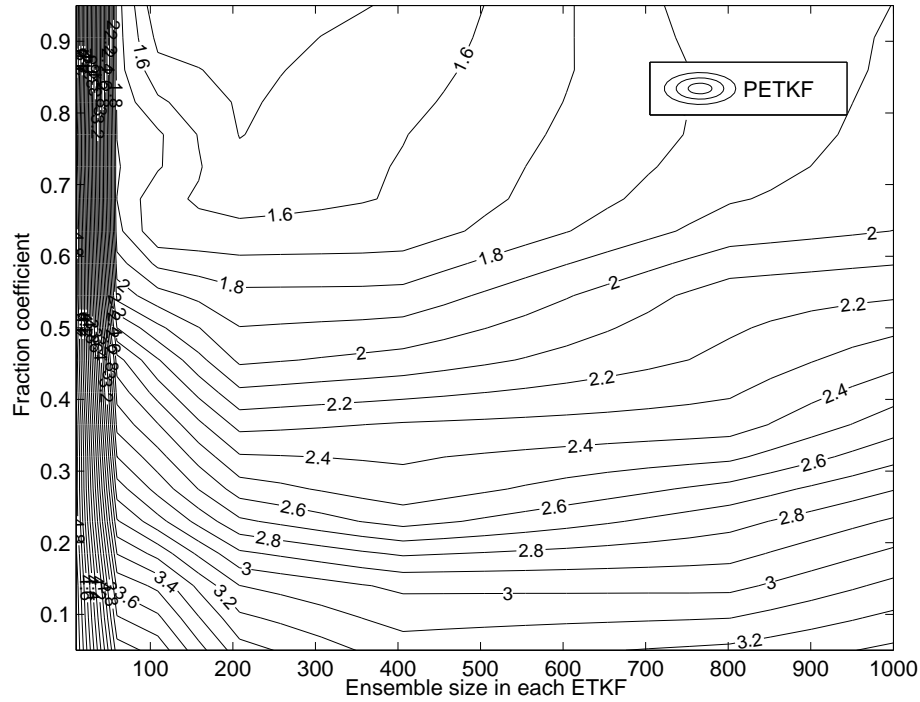


Figure 3: RMS errors (over 20 experiments) of the stochastic EnKF and the ETKF as the functions of the ensemble size.



(a) Stochastic EnKF-based PKF



(b) ETKF-based PKF

Figure 4: RMS errors (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed number of Gaussian *pdfs* of 3 in each PKF) as the functions of the fraction coefficient and the ensemble size of the ensemble filter.

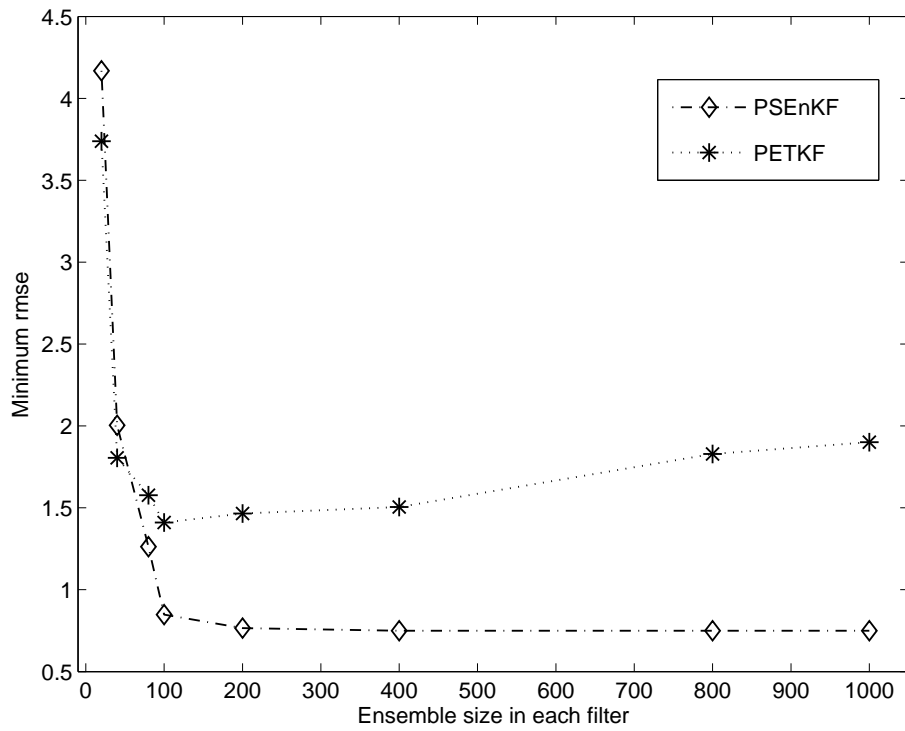
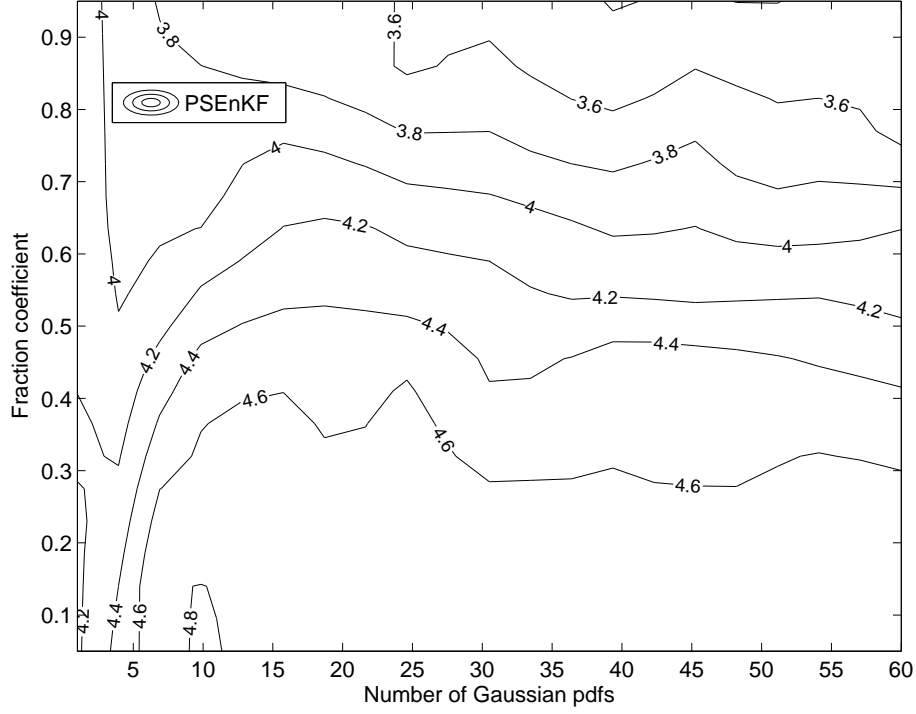
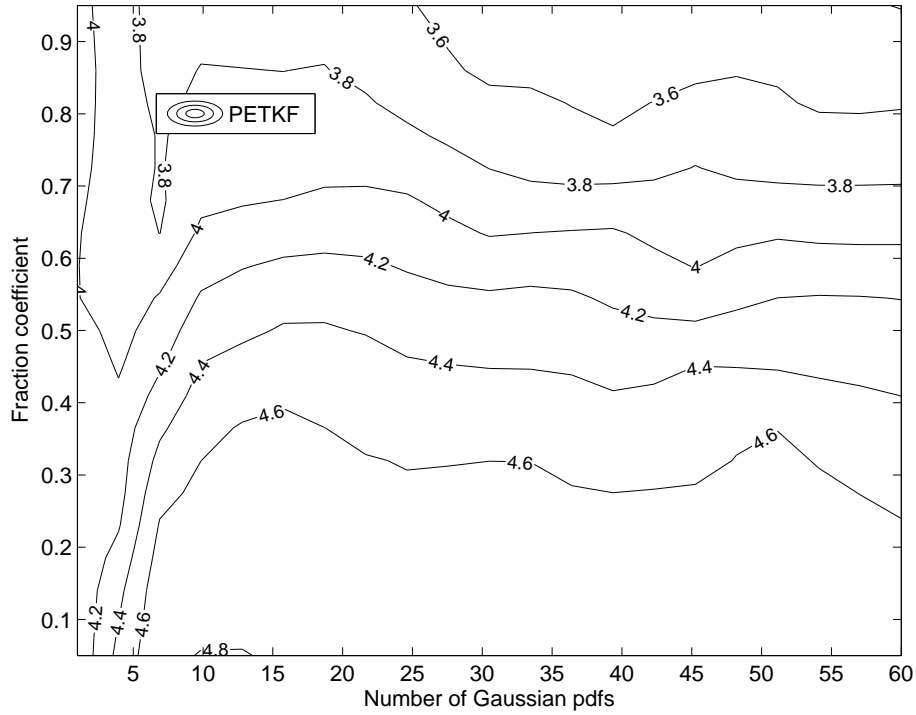


Figure 5: Minimum rms errors \hat{e}_{min} (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed number of Gaussian *pdfs* of 3 in each PKF) as the function of the ensemble size in each ensemble filter.



(a) Stochastic EnKF-based PKF



(b) ETKF-based PKF

Figure 6: RMS errors (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed ensemble size of 20 in each ensemble filter) as the functions of the fraction coefficient and the number of Gaussian *pdfs* in the MON.

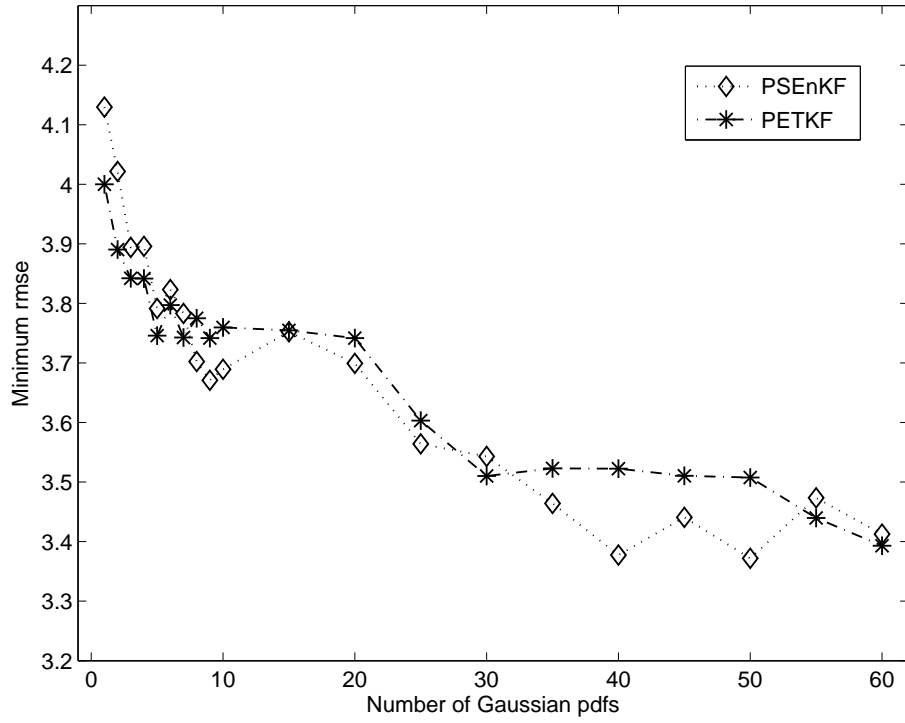


Figure 7: Minimum rms errors \hat{e}_{min} (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed ensemble size of 20 in each ensemble filter) as the function of the number of Gaussian *pdfs* in the MON.

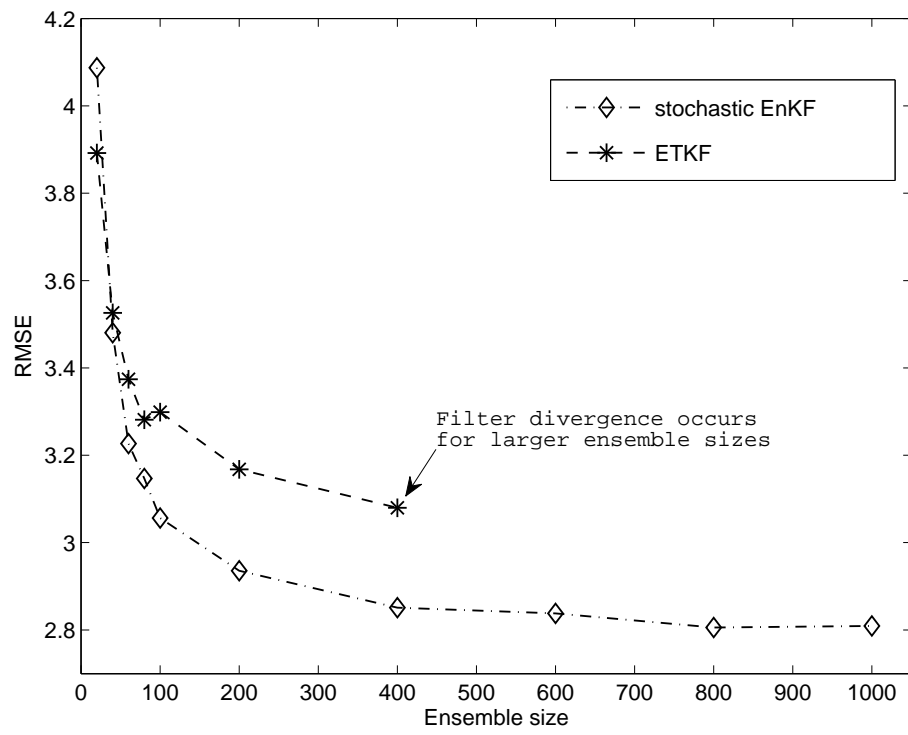
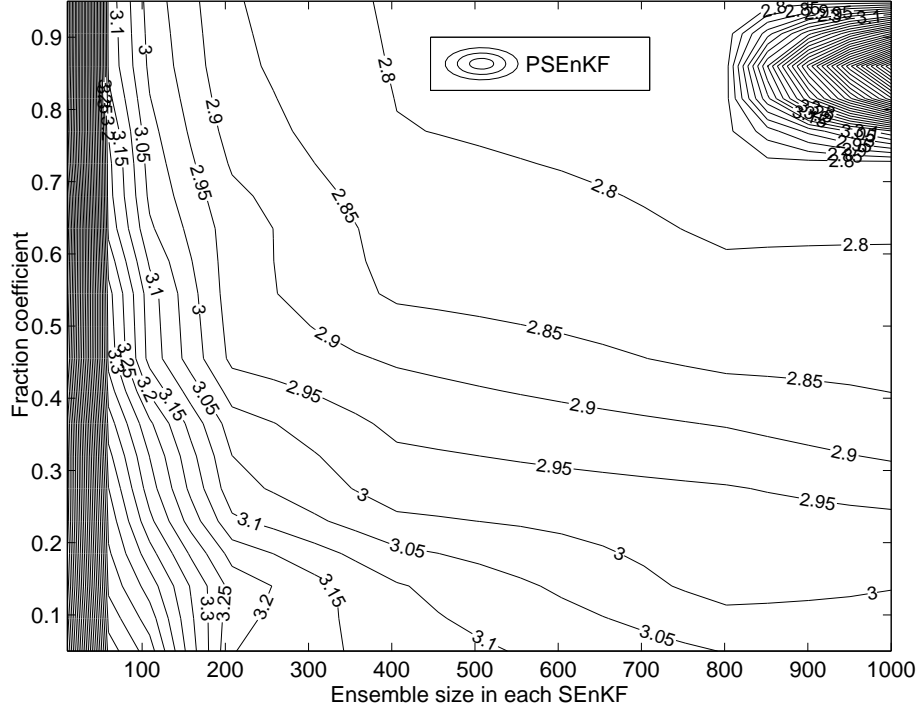
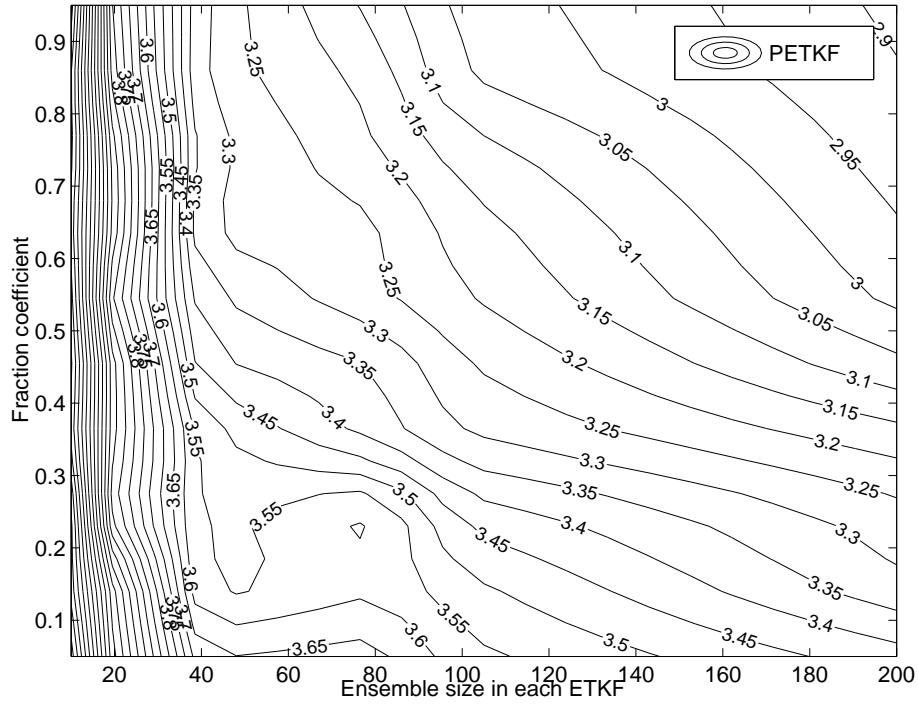


Figure 8: RMS errors (over 20 experiments) of the stochastic EnKF and the ETKF as the functions of the ensemble size.



(a) Stochastic EnKF-based PKF



(b) ETKF-based PKF

Figure 9: RMS errors (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed number of Gaussian *pdfs* of 3 in each PKF) as the functions of the fraction coefficient and the ensemble size of the ensemble filter. In Fig. 9(b)

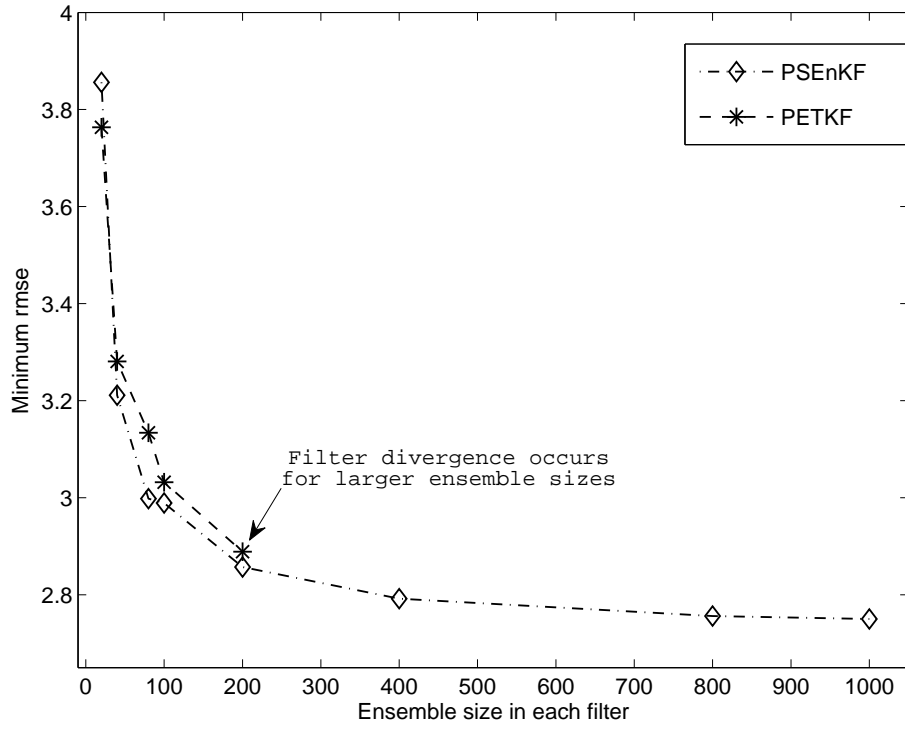


Figure 10: Minimum rms errors \hat{e}_{min} (over 20 experiments) of the stochastic EnKF- and ETKF-based PEnKFs (with a fixed number of Gaussian *pdfs* of 3 in each PKF) as the function of the ensemble size in each ensemble filter.

Support Material: The Full Re-sampling

Algorithm

Here we discuss how to construct the ensemble set $\{\mathbf{X}_{en}^i, i = 1, \dots, q\}$ in the PEnKF.

We note that the relative positions of the dimension n of the random vector \mathbf{x} , the number q of the Gaussian *pdfs* in the MON Eq. (13), and the ensemble size m of each EnKF in the PKF determines our re-sampling strategies. In certain circumstances, a singular value decomposition (SVD) may be required on the covariance matrix $\bar{\mathbf{P}}$ in Eq. (14) such that

$$\bar{\mathbf{P}} = \mathbf{V}\mathbf{D}\mathbf{V}^T = \sum_{i=1}^n \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T, \quad (\text{S.1})$$

where \mathbf{V} is the matrix consisting of the eigenvectors \mathbf{e}_i of \bar{P} , and $\mathbf{D} \equiv \text{diag}(\sigma_1^2, \dots, \sigma_n^2)$ the diagonal matrix consisting of the corresponding eigenvalues σ_i^2 (we also assume $\sigma_i \geq 0$ without loss of generality). Depending on the values of q , m and n , one may avoid computing the full spectra of $\bar{\mathbf{P}}$, as to be shown below.

Case I: $q \leq n$ and $m \leq n$

In this case the number q of (re-approximation) Gaussian distributions and the ensemble size m are both less than the dimension n of the system state. We consider two possibilities below.

1. $q \leq m \leq n$

Here we choose

$$\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}}) (\theta_i - \bar{\mathbf{x}})^T = (1 - c^2) \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T, \quad (\text{S.2a})$$

$$\Phi = c^2 \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T + \sum_{i=q}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T. \quad (\text{S.2b})$$

810 The reason to choose the superscripts $q - 1$ and $m - 1$ on the right hand side of
 811 Eqs. (S.2a) and (S.2b) will be made clear soon. We also note that the sum

$$\Phi + \frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}}) (\theta_i - \bar{\mathbf{x}})^T = \sum_{i=1}^{n-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T \quad (\text{S.3})$$

812 is not equal to $\bar{\mathbf{P}}$ exactly. Instead, it only adds up to the first $(m - 1)$ terms of $\sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T$.

813 Let $\Theta = [\theta_1, \dots, \theta_q]$ be the collection of the means θ_i in the MON $\tilde{p}(\mathbf{x})$, and

$$\mathbf{S}_\mu = \sqrt{1 - c^2} [\sigma_1 \mathbf{e}_1, \dots, \sigma_{q-1} \mathbf{e}_{q-1}]$$

814 be the square root of $(1 - c^2) \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T$ in Eq. (S.2a), then it can be verified that

$$\Theta = \bar{\mathbf{x}} \mathbf{1}_q^T + \sqrt{q} \mathbf{S}_\mu \mathbf{C}_{q-1,q} \quad (\text{S.4})$$

815 yields a set of the means θ_i that satisfy Eq. (S.2a), where $\mathbf{1}_q^T$ denotes the transpose
 816 of the $q \times 1$ column vector $\mathbf{1}_q$ with all its elements being one (so that $\bar{\mathbf{x}} \mathbf{1}_q^T$ consists
 817 of N identical column vectors $\bar{\mathbf{x}}$), and $\mathbf{C}_{q-1,q}$ is a $(q - 1) \times q$ matrix satisfying that
 818 $\mathbf{C}_{q-1,q}(\mathbf{C}_{q-1,q})^T = \mathbf{I}_{q-1}$, with \mathbf{I}_{q-1} being the $(q - 1)$ -dimensional identity matrix,
 819 and that $\mathbf{C}_{q-1,q} \mathbf{1}_q = \mathbf{0}_{q-1}$, with $\mathbf{0}_{q-1}$ being a $(q - 1) \times 1$ column vector with all its
 820 elements being zero. The first constraint, $\mathbf{C}_{q-1,q}(\mathbf{C}_{q-1,q})^T = \mathbf{I}_{q-1}$ guarantees that the
 821 sample covariance of Θ satisfies the constraint in Eq. (S.2a), and the second one,
 822 $\mathbf{C}_{q-1,q} \mathbf{1}_q = \mathbf{0}_{q-1}$ guarantees that the sample mean of Θ is equal to $\bar{\mathbf{x}}$, as is required
 823 in Eq. (16). For the generation of such a matrix $\mathbf{C}_{q-1,q}$, readers are referred to,
 824 for example, Hoteit et al. (2002); Pham (2001). In addition, since the dimension of
 825 $\mathbf{C}_{q-1,q}$ is $(q - 1) \times q$, we require that the dimension of the square root matrix \mathbf{S}_μ is
 826 $n \times (q - 1)$. Therefore, on the right hand side of Eq. (S.2a), the superscript shall be
 827 $(q - 1)$, rather than q . The reason to use the superscript $(m - 1)$ in Eq. (S.2b) is
 828 similar, as can be seen below.

829 To generate the ensembles \mathbf{X}_{en}^i ($i = 1, \dots, q$), with θ_i and Φ being their sample
 830 means and covariances, we first construct the square root matrix

$$\mathbf{S}_\phi = [c\sigma_1 \mathbf{e}_1, \dots, c\sigma_{q-1} \mathbf{e}_{q-1}, \sigma_q \mathbf{e}_q, \dots, \sigma_{n-1} \mathbf{e}_{m-1}] \quad (\text{S.5})$$

831 of Φ , and generate \mathbf{X}_{en}^i by

$$\mathbf{X}_{en}^i = \theta_i \mathbf{1}_m^T + \sqrt{m} \mathbf{S}_\phi \mathbf{C}_{m-1,m}, \text{ for } i = 1, \dots, q, \quad (\text{S.6})$$

832 where $\mathbf{C}_{m-1,m}$ is a matrix similar to $\mathbf{C}_{q-1,q}$ in Eq. (S.4). We note that the term
 833 $\sqrt{m} \mathbf{S}_\phi \mathbf{C}_{m-1,m}$ is common to all EnKFs, and thus only needs to be calculated once.
 834 This is direct implication from the choice of the uniform covariance Φ in $\tilde{p}(\mathbf{x})$, as we
 835 have pointed out previously, which leads to computational savings in comparison to
 836 the non-uniform choice.

837 2. $m < q \leq n$

Here we choose

$$\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}}) (\theta_i - \bar{\mathbf{x}})^T = (1 - c^2) \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T + \sum_{i=m}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T, \quad (\text{S.7a})$$

$$\Phi = c^2 \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T. \quad (\text{S.7b})$$

838 Now define the square root matrix

$$\mathbf{S}_\mu = [\sqrt{1 - c^2} \sigma_1 \mathbf{e}_1, \dots, \sqrt{1 - c^2} \sigma_{m-1} \mathbf{e}_{m-1}, \sigma_m \mathbf{e}_m, \dots, \sigma_{q-1} \mathbf{e}_{q-1}] \quad (\text{S.8})$$

839 of the term on right hand side of Eq. (S.7a), and the square root matrix

$$\mathbf{S}_\phi = c [\sigma_1 \mathbf{e}_1, \dots, \sigma_{n-1} \mathbf{e}_{m-1}] \quad (\text{S.9})$$

840 of Φ in Eq. (S.7b). Then θ_i and \mathbf{X}_{en}^i can be generated through Eqs. (S.4) and (S.6),
 841 respectively.

842 **Case II: $q \leq n$ and $m > n$**

In this case the number q of Gaussian distributions is less than the dimension n of the system state, but the ensemble size m is larger than n . We choose

$$\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}}) (\theta_i - \bar{\mathbf{x}})^T = (1 - c^2) \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T, \quad (\text{S.10a})$$

$$\mathbf{\Phi} = c^2 \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T + \sum_{i=q}^n \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T = \bar{\mathbf{P}} - (1 - c^2) \sum_{i=1}^{q-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T. \quad (\text{S.10b})$$

843 The last equality in Eq. (S.10b) implies that one does not need to compute the full
844 spectra of $\bar{\mathbf{P}}$ and the corresponding eigenvectors. Instead, one only needs to compute
845 the first $(q - 1)$ terms of $\sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T$.

846 Now define the square root matrix

$$\mathbf{S}_\mu = \sqrt{1 - c^2} [\sigma_1 \mathbf{e}_1, \dots, \sigma_{q-1} \mathbf{e}_{q-1}], \quad (\text{S.11})$$

847 so that one can again adopt Eq. (S.4) to generate θ_i ($i = 1, \dots, q$). To generate the
848 ensembles \mathbf{X}_{en}^i , the situation here is different from that in the previous case, in that
849 the ensemble size m is larger than the dimension n , so that one cannot obtain enough
850 ensemble members through Eq. (S.6). As a result, one may instead choose to draw
851 $(m - 1)$ samples $\delta \mathbf{x}_j^\phi$ ($j = 1, \dots, m - 1$) from the distribution $N(\delta \mathbf{x} : \mathbf{0}_n, \mathbf{\Phi})$ to form
852 a matrix $\Delta \mathbf{X}_\phi \equiv [\delta \mathbf{x}_1^\phi, \dots, \delta \mathbf{x}_{m-1}^\phi]$. Then the ensemble \mathbf{X}_{en}^i is produced via

$$\mathbf{X}_{en}^i = \theta_i \mathbf{1}_m^T + \Delta \mathbf{X}_\phi \mathbf{C}_{m-1,m}, \quad \text{for } i = 1, \dots, q. \quad (\text{S.12})$$

853 Eq. (S.12) is similar to the partial re-sampling scheme in Hoteit et al. (2008), although
854 here the perturbation term $\Delta \mathbf{X}_\phi \mathbf{C}_{m-1,m}$ can be common to all EnKFs, and thus can
855 be drawn only once to reduce computational cost.

856 **Case III: $q > n$ and $m \leq n$**

In this case the ensemble size m is no larger than the dimension n of the system state, but the number q of Gaussian distributions is. We choose

$$\frac{1}{q} \sum_{i=1}^q (\theta_i - \bar{\mathbf{x}}) (\theta_i - \bar{\mathbf{x}})^T = (1 - c^2) \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T + \sum_{i=m}^n \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T = \bar{\mathbf{P}} - c^2 \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T, \quad (\text{S.13a})$$

$$\Phi = c^2 \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T. \quad (\text{S.13b})$$

857 Since $q > n$, we choose to draw $(q - 1)$ samples $\delta \mathbf{x}_j^\mu$ from the distribution $N(\delta \mathbf{x} :$
 858 $\mathbf{0}_n, \bar{\mathbf{P}} - c^2 \sum_{i=1}^{m-1} \sigma_i^2 \mathbf{e}_i \mathbf{e}_i^T)$ to form a matrix $\Delta \mathbf{X}_\mu \equiv [\delta \mathbf{x}_1^\mu, \dots, \delta \mathbf{x}_{q-1}^\mu]$, while θ_i are gener-
 859 ated by

$$\Theta = \bar{\mathbf{x}} \mathbf{1}_q^T + \Delta \mathbf{X}_\mu \mathbf{C}_{q-1, q}. \quad (\text{S.14})$$

860 Let

$$\mathbf{S}_\phi = c[\sigma_1 \mathbf{e}_1, \dots, \sigma_{m-1} \mathbf{e}_{m-1}], \quad (\text{S.15})$$

861 then \mathbf{X}_{en}^i can be generated through Eq. (S.6).

862 **Case IV: $q > n$ and $m > n$**

863 In this case both the number q of Gaussian distributions and the ensemble size m
 864 are larger than the dimension n of the system state. We let $\Phi = c^2 \bar{\mathbf{P}}$ and define
 865 $\mathbf{P}_n = (1 - c^2) \bar{\mathbf{P}}$. To generate θ_i , we first draw $(q - 1)$ samples $\delta \mathbf{x}_j^\mu$ from the distribution
 866 $N(\delta \mathbf{x} : \mathbf{0}_n, \mathbf{P}_n)$ to form a matrix $\Delta \mathbf{X}_\mu = [\delta \mathbf{x}_1^\mu, \dots, \delta \mathbf{x}_{q-1}^\mu]$, and then apply Eq. (S.14).
 867 Meanwhile, we also draw $(m - 1)$ samples $\delta \mathbf{x}_j^\phi$ from the distribution $N(\delta \mathbf{x} : \mathbf{0}_n, \Phi)$ to
 868 form a matrix $\Delta \mathbf{X}_\phi \equiv [\delta \mathbf{x}_1^\phi, \dots, \delta \mathbf{x}_{m-1}^\phi]$, and then apply Eq. (S.12) to generate the
 869 ensembles \mathbf{X}_{en}^i .

